ETCHING SIMULATION OF NONPLANAR LAYERS IN THE SAMPLE PROGRAM

by

Stephen F. Meier

Memorandum No. UCB/ERL M87/41

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Chapter 1

Introduction

With the increasing complexity of VLSI circuits , device interconnection plays a greater role. Multilevel metalization is necessary for interconnecting the large number of devices on a chip and is a dominant factor in determining chip speed, power and size. Integrated circuit processes have been extended to form the additional metal and dielectric layers required for multiple level metalization. These process extensions have increased process complexity as evidenced by an increased number of process steps and decreased planarity of wafer topography. To handle this complexity and to predict process windows, engineers require sophisticated simulation tools.

A critical procedure in the metallization process is selective removal of material from the surface of the wafer. This process is referred to as etching and is simulated in a portion of the SAMPLE program. Previously, the etching machine in the SAMPLE program was unable to simulate process steps of great complexity due to the restriction of planar underlying layers. Simulation capabilities were limited to examples having only flat layers of material below the top most layer. In the new version of the etching machine, the user is allowed to specify any arbitrary profile for all underlying layers. This report discusses the extension of the SAMPLE etching machine to nonplanar layers and presents several examples of the enhanced capability.

Chapter 2

Algorithm Description

2.1 Previous Work on Etching Simulation in SAMPLE

SAMPLE 1,2 is a FORTRAN program which is capable of simulating the time evolution of topographical features of Integrated Circuit devices during multiple process steps. Within the etching machine of the SAMPLE program the process steps are isotropic deposition, isotropic (wet) etching and plasma (dry) etching.

The etching machine uses a string point model to simulate the advancement of the top profile during a process step. In this model, a profile describing the top surface of a semiconductor layer is divided into small segments. At each iteration of the simulation, an advancement vector is calculated for each of the string points. For calculation of the distance and direction of a point's vector, an etch rate is required. The etch rate is determined by using the layer of the point to index into a table of rates. The determination of a point's layer is the main change in the advancement algorithm.

Previously, the SAMPLE etching machine allowed only planar underlying layers. The layer of a point was determined by a linear comparison with layer thicknesses. If the z value of the point was less than a layer thickness from the substrate, an intersection with that layer occurred. In the new version, the underlying layers have nonplanar profiles therefore a more rigorous intersection checking algorithm was required.

2.2 Algorithm Summary

The methodology, in the new version, is to determine which layer each point is located in before the advancement calculation begins. The intersection algorithm traverses the top profile and at each point tests for an intersection with bounding profiles of the current layer. At the start of the traversal, the starting layer is determined by a linear comparison between the left boundary point of the top profile with the boundary points of the underlying layers using a linear comparison. Next, the algorithm proceeds to the following top profile point and performs an intersection check with the current layer profile boundaries. At an intersection point, the current layer is updated and the algorithm continues with the next point of the top profile. This procedure is repeated for every point in the profile. An effort is made to bound the intersection search through comparisons of a profile point's location with that of the boundary segments.

2.3 Data Structure Modifications

The nonplanar algorithm requires additional storage. For maintenance of the layer number of each profile point, the IXZLAY array has been created. This array acts as a record field, storing the layer number for each point in the XZ profile point array. In addition, the two dimensional array UXZ was added to provide storage for the underlaying arrays. This array stores the profile points for each of the underlying layers.

2.4 Intersection Check

An intersection check is performed between each profile point and the bounding profiles of its layer. In this check, both the current and previous profile point (XZCUR,XZPRV) are used for comparison with the current and previous profile points of the underlying layer (UXZCUR,UXZPRV). The intersection check proceeds by iterating through each of the line segments that compose the layer boundary. For each segment, a linear comparison is performed with the x and y values of the endpoints to determine if an intersection if possible. If the test succeeds, it is determined which of four cases the segments are associated with. The cases correspond to different orientations of segment endpoints with each other and are enumerated in Figure 1. For each case, there are two segment endpoints which occur within the x range of the opposing segment (marked as □ in Figure 1). The z intercepts of these points with their opposing segments are calculated (marked as •). Next, a linear comparison is made between the the z locations of the segment endpoints and their corresponding z intercepts. If the comparison result for both points is different, then an intersection occurs, otherwise there is no intersection. As shown in Figure 2 , there are cases in which more than a single intersection can occur. Therefore, a count of the intersections is maintained and when the underlying profile segments have been exhausted an odd count indicates a layer change.

2.5 Bounding the Search for Monotonic Profiles

The intersection checking algorithm iterates through each segment of a profile searching for an intersection. A search of the i'th layer has complexity on the order of $N_{top}*N_i$ where N_{top} is the number of points in the top profile and N_i is the number of points in the i'th underlying layer. In the case of a monotonic underlying layer, we can prune the search space. The definition of a monotonic profile is a profile which conforms to the following property: $x_1 < x_2 \cdots < x_n$. With such a profile, the search can be terminated once the x value of the current top profile point is passed by the x value of the current underlying profile point. For non-monotonic profiles all the underlying segments of a profile must be searched. The etching machine automatically determines if any of the underlying layers or the top profile are monotonic. If the top profile becomes non-monotonic after an advancement step the program will detect the change and modify the search space accordingly.

Chapter 3

Input Format Description

3.1 Profile Description

The extension of the etching machine to handle nonplanar layers has prompted the redefinition of the NONPLANAR (TRIAL 96) statement. The new format takes on the following form.

$$\text{NONPLANAR} \quad \text{Layer\#} \quad (x_1,y_1) \; (x_2,y_2) \; \cdots \; (x_n,y_n)$$

Here the layer numbering conforms to the same numbering scheme as previous versions of the etching machine where N is the total number of layers (0=substrate, N-1=Top Layer) with maximum N of 5 in version 1.7. The top profile is still specified with the ETCHPROFILE statement. Currently, the number of points in the profile (n) is limited to 249 points in version 1.7. The NONPLANAR statement must be preceded by the ETCHLAYERS statement indicating the number of layers in the structure. Additionally, use of the ETCHLAYERS statement for layer width specification is superseded by inclusion of a NONPLANAR statement. The plot scaling for the z axis is performed automatically within the modified program. The scaling routine estimates the maximum etch distance using the product of the etching time with the maximum etch rate, therefore any profile is guaranteed to fit within the window. Also, with a NONPLANAR statement specified, all layers must be listed as NONPLANAR (ie. there can be no intermixing of the ETCHLAYERS statement with the NONPLANAR statement). One limitation on the input structure is that no isolated structures are allowed. Each layer must extend across the entire simulation window. This problem can be circumvented by matching profiles with the the profile of the layer below thus having a layer with zero thickness in parts. This method was used in the input structure of the oxide spacer process presented in the example chapter of this report.

3.2 Multi-Step Capability

The new version of the etching machine has the capability to simulate multi-step processes. After an isotropic deposition, the previous top profile is shifted into the first underlying profile and the previous underlying profiles are shifted down in the UXZ array. This capability is demonstrated with the oxide spacer process which is presented in the example chapter of this report.

Chapter 4

Algorithm Limitations and Areas For Future Work

4.1 Advancement Error

An inherent problem in the string model algorithm is controlling advancement into layers of differing etch rates. The advancement algorithm uses an etching rate based on the layer determined in the previous advancement iteration. Therefore, a point which is about to enter a layer with a differing etch rate will have an inaccurate advancement vector. The error is proportional to Time Step Size * Difference in Etch Rates. To reduce this error the algorithm could be modified to use very small time steps for each advancement or to perform the advancement in two passes. In the first pass, the algorithm could determine if an intersection will occur and then modify the time step to advance the string points only as far as the nearest intersection. Either modification would severely increase the execution time of the program.

4.2 Boundary Condition Inaccuracies

Another limitation of the etching machine occurs with the handling of boundary conditions. When a profile point intersects with a layer, its etch rate is modified and the program uses that etch rate in the next advancement calculation. This situation can leave a segment split with two endpoints in different layers. Then, as the advancement continues the segment movement is inaccurate. This problem is quite apparent in the first metal lift-off simulation presented in the example chapter. The undercutting profile is slowed near the boundary resulting in a non-physical curved profile. A solution to correct this problem would be to scan the profile for intersections and insert points at the boundary point. This would ensure that each segment resides completely within one layer.

4.3 Iteration Time Step Selection

Both the past and new versions of the etching machine both suffer from an improperly controlled iteration time step size. The program determines a time step based on the total time, the accuracy parameter and the time between plot outputs. This results in very poor rates of the top layers were matched exactly resulting in a planar surface. In the second example, the SiO_2 film etches slower than surface photoresist layer which causes pillar formation in the location of the original depression. Lastly, in the third example, the relative etch rates are reversed and it is seen that a reduced slope depression results.

To demonstrate that the new version can simulate overhanging structures the input profile in Figure 7 was etched. For this example, the deposition machine of SAMPLE was used to sputter the aluminum over the oxide steps. Then a horizontal profile was sketched over the profile to mimic the deposition of spin-on glass. Two simulations were performed. In the first simulation, only the spin-on glass was etched. The resulting profile is shown in Figure 8. In the second simulation, both the aluminum (.0035 $\frac{um}{sec}$) and spin-on glass (.0015 $\frac{um}{sec}$) layers were etched simultaneously. In Figure 9, the resulting profile is presented.

5.2 Example 2: Oxide Spacer Formation - A Multi-Step Simulation

A few advanced MOS processes include steps to form oxide spacers which improve isolation between the gate and drain regions. In this example, the entire oxide spacer formation process is simulated. The initial structure is that of a basic MOS process as shown in Figure 10. In the first process step, an oxide film is formed using chemical vapor deposition. This step is simulated using isotropic deposition. Next, a plasma etch step removes material in a directional fashion to form the shape of the spacer. Plasma etching is simulated using a fully anisotropic etch. Lastly , a wet etch is used to decrease the size of the spacer uniformly. This last process step is simulated using an isotropic etch. The results of the simulation are presented in Figures 11,12 and 13. It can be seen that the isotropic etching step is not required to form the oxide spacer yet it was included to demonstrate the ability to simulate multiple etching and isotropic deposition steps.

5.3 Example 3: Additive High Resolution Metal Lift-Off

A recently proposed method of metallization uses a lift-off process to pattern features using only isotropic etching.[5] In the lift-off process, a photoresist film is deposited and patterned with a reversed polarity to that of the desired metal film. Next, the metal is deposited over the entire wafer surface. This is followed by a spin of a second photoresist layer. The lift-off process takes advantage of the fact that the spun-on film is thinest in the region that passes over the original photoresist step as shown in Figure 14. The etching portion of the lift-off process, is a two step procedure. First, the top photoresist layer is etched so that a break is formed around the step area. Then, the aluminum is etched through the break until the first photoresist layer is exposed. Finally, the first photoresist is removed by an acetone bath.

In this example, the etching portion of the metal lift-off process is simulated. The first simulation step, is a fully selective etch of the top layer photoresist to reveal the aluminum film as shown in the resulting profile (Figure 15). In the second simulation step, the aluminum is etched with complete selectivity to the other films. In the resulting profile (Figure 16), it is seen that the aluminum is patterned successfully.

To demonstrate the capability of the new etching machine to simulate overhanging profiles an extreme profile structure was simulated. The initial profile as shown in Figure 17 has an overhanging aluminum layer. Note that this profile was sketched by hand and does not closely resemble any physical structure but demonstrates the ability of the program to handle severe geometry. As shown in the resulting profiles (Figures 18,19), the program handles the overhanging profile successfully and is even able to simulate the undercutting of the top photoresist layer. In the second step, the remaining photoresist layer is undercut on both sides by the etching of the aluminum. When the undercutting is complete, the isolated structure has been removed and the two sides of the profile join. The top profile then continues to advance into the aluminum layer below the original photoresist structure.

Chapter 6

Conclusion

Extensions to the etching machine of the SAMPLE program have been completed. The extended program can simulate etching and isotropic deposition with multiple arbitrary non-planar profiles. An algorithm to detect intersections between multiple profile boundaries was developed. Within the algorithm, there are tests to detect monotonic profiles which enable bounding of profile searches. Limitations of the program with respect to boundary conditions and time step determination were discussed. Also indicated, was the problem of inter-module communication with multiple layer profiles. The enhanced program was used to simulate several process sequences from multi-level metalization processes. Spin-on and etch-back planarization was simulated using various etch rates and layer topography. An oxide spacer process using a sequence of deposition and etching steps was presented. Additionally, a high resolution additive lift-off process using two cycles of isotropic etching was simulated. In these examples, the ability of the etching machine to simulate overhanging profiles was demonstrated.

References

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3. V. Grewal, A. Gschwandtner, and G. Higelin, "A Novel Multilevel Metalization Technique For Advanced CMOS and Bipolar Integrated Circuits," *Proceedings IEEE VLSI Multilevel Interconnection Conference*, p. 107,113, June 1986.

4. Pat Elkins, Karen Reinhardt, and Rebecca Tang, "A Planarization Process For Double Metal CMOS Using Spin-On-Glass as a Sacrificial Layer," *Proceedings IEEE VLSI Multilevel Interconnection Conference*, p. 100,106, June 1986.

5. Pei-lin Pai, Yosi Shacham-Diamand, and William G. Oldham, "A High Resolution Lift-Off Technology for VLSI Interconnections," *Proceeding IEEE VLSI Multilevel Interconnection Conference*, p. 205,211, June 1986.

Figure 1 : Intersection Check Cases

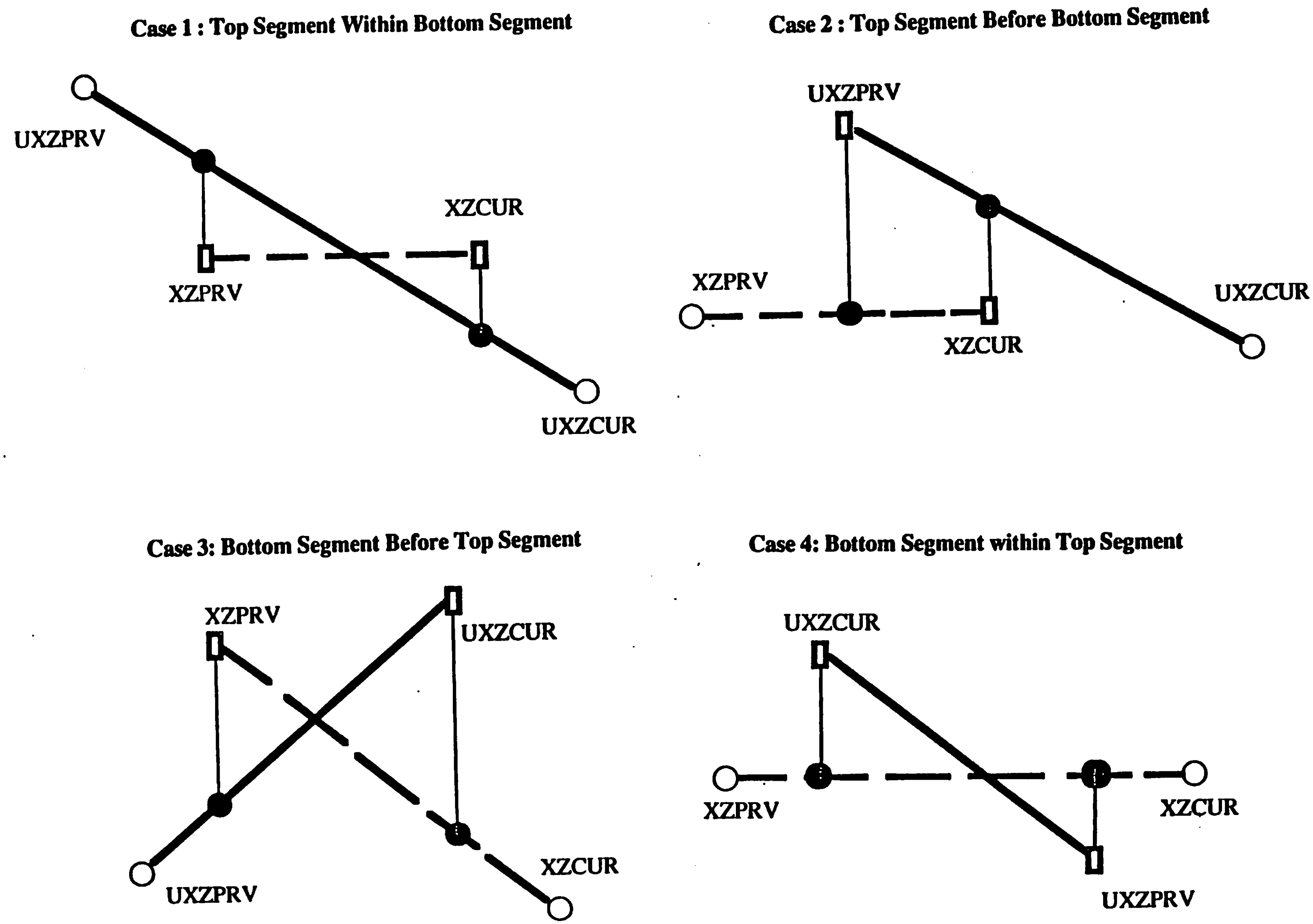


Figure 2: Multiple Intersection Example

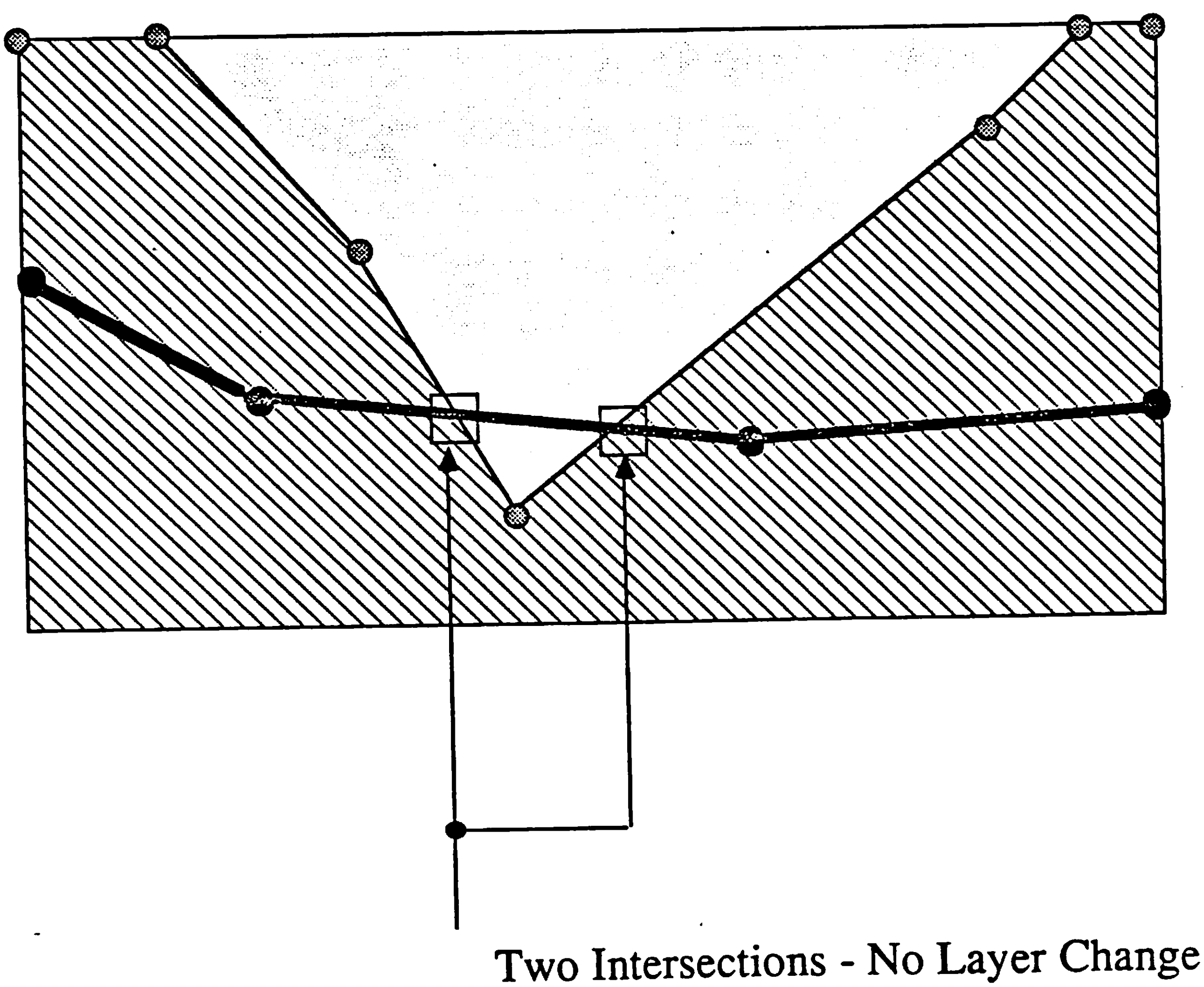


Figure 3: Initial Etch-Back Planarization Structure

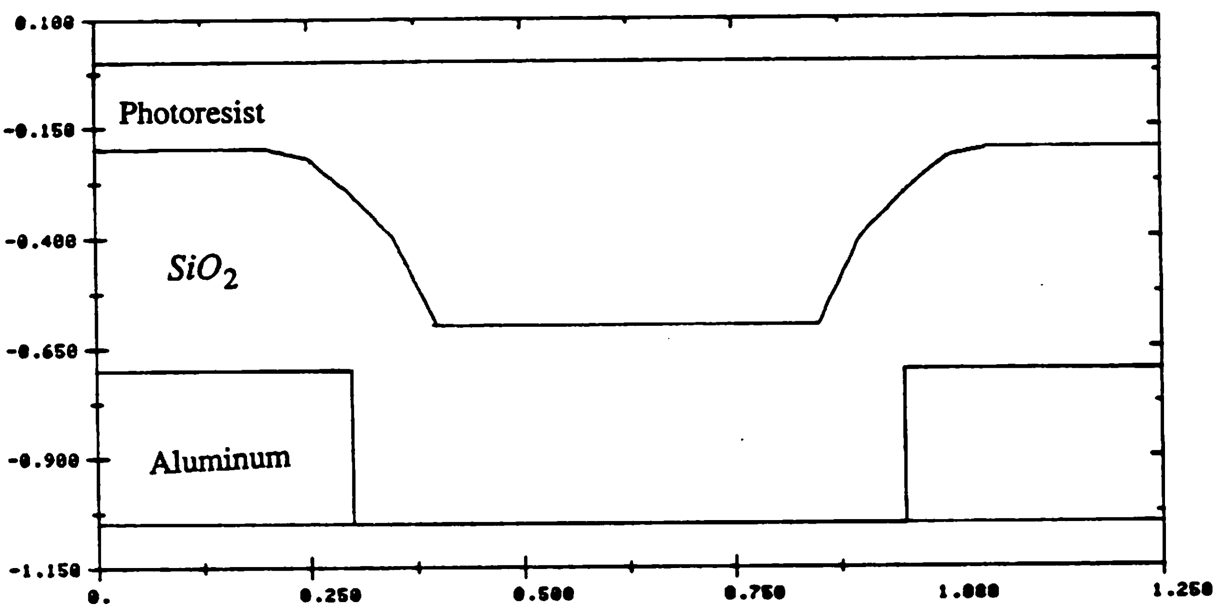
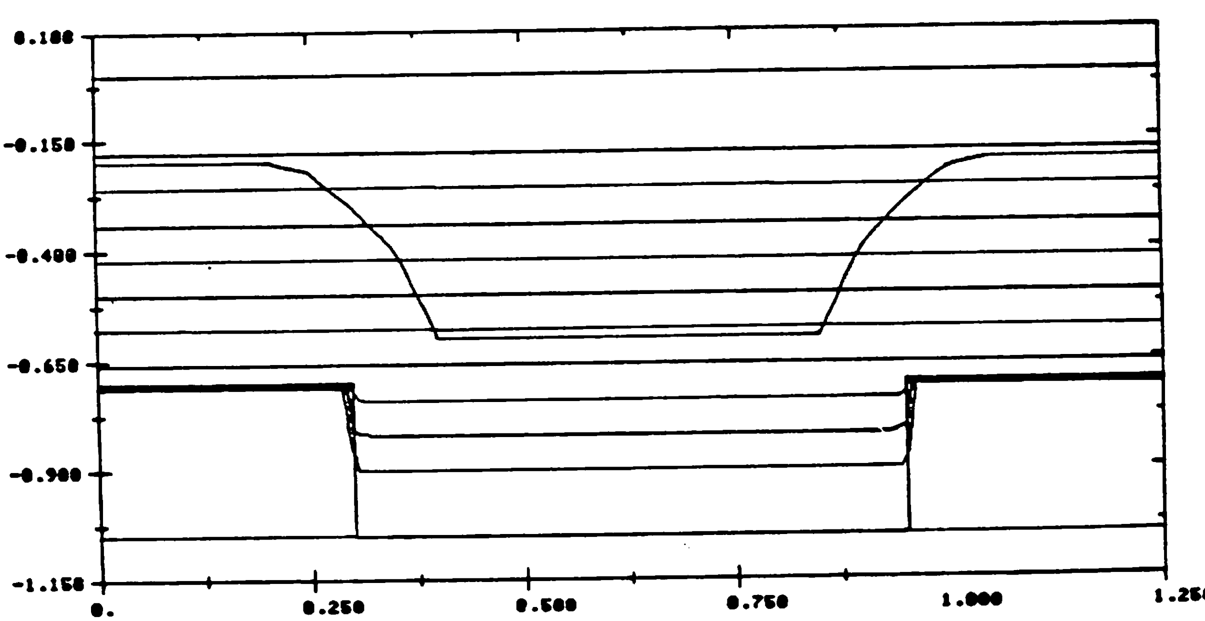


Figure 4: Etch-Back Planarization With Equal Rates



Rates:

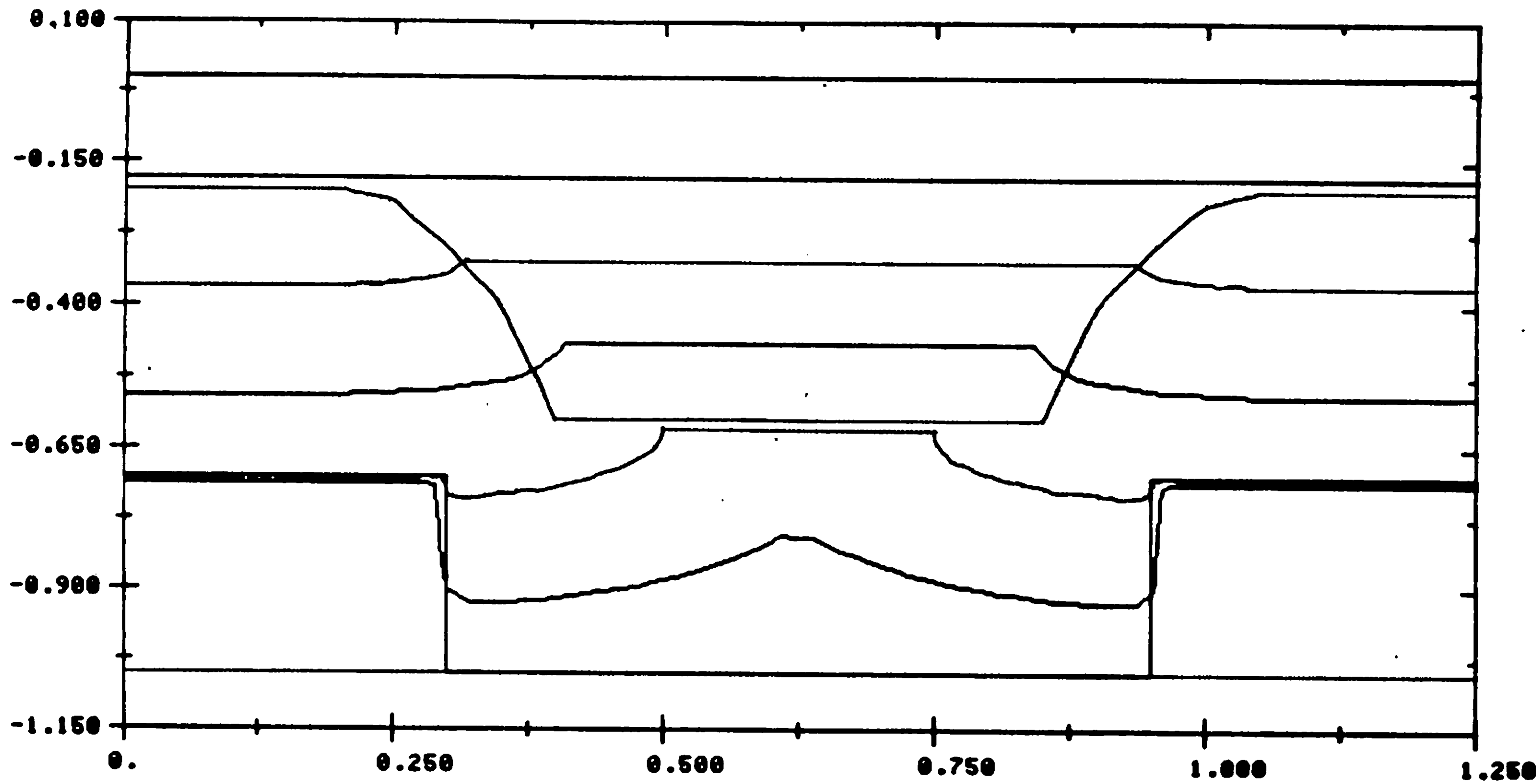
$SiO_2 = .002 \frac{um}{sec}$

$Photoresist = .002 \frac{um}{sec}$

$Aluminum = .0001 \frac{um}{sec}$

$Substrate = .0001 \frac{um}{sec}$

Figure 5: Etch-Back Planarization



Rates:

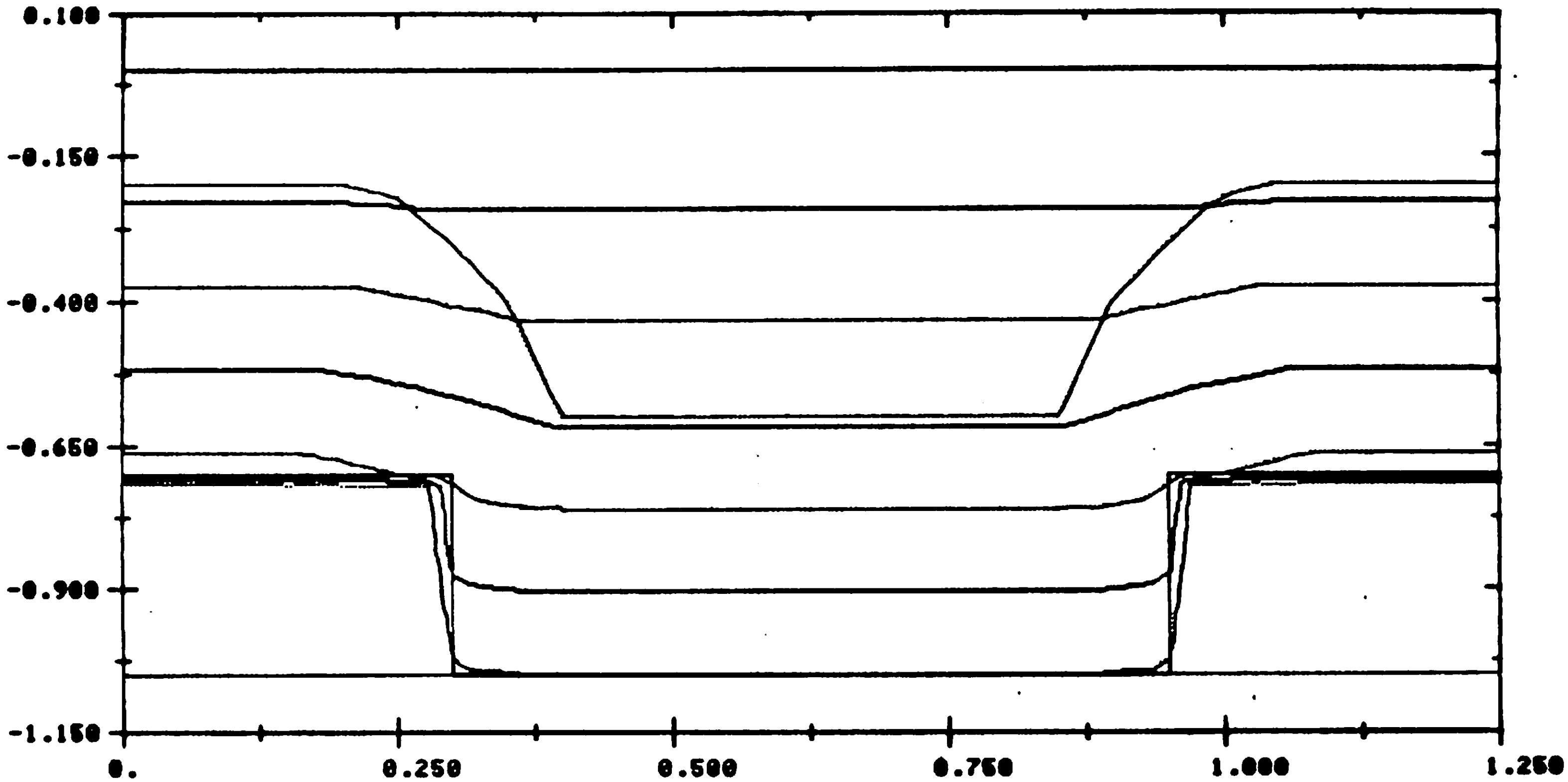
$SiO_2 = .002 \frac{um}{sec}$

$Photoresist = .0015 \frac{um}{sec}$

$Aluminum = .0001 \frac{um}{sec}$

$Substrate = .0001 \frac{um}{sec}$

Figure 6: Etch-Back Planarization



Rates:

$SiO_2 = .0015 \frac{um}{sec}$

$Photoresist = .002 \frac{um}{sec}$

$Aluminum = .0001 \frac{um}{sec}$

$Substrate = .0001 \frac{um}{sec}$

Figure 7: Initial Overhanging Planarization Structure

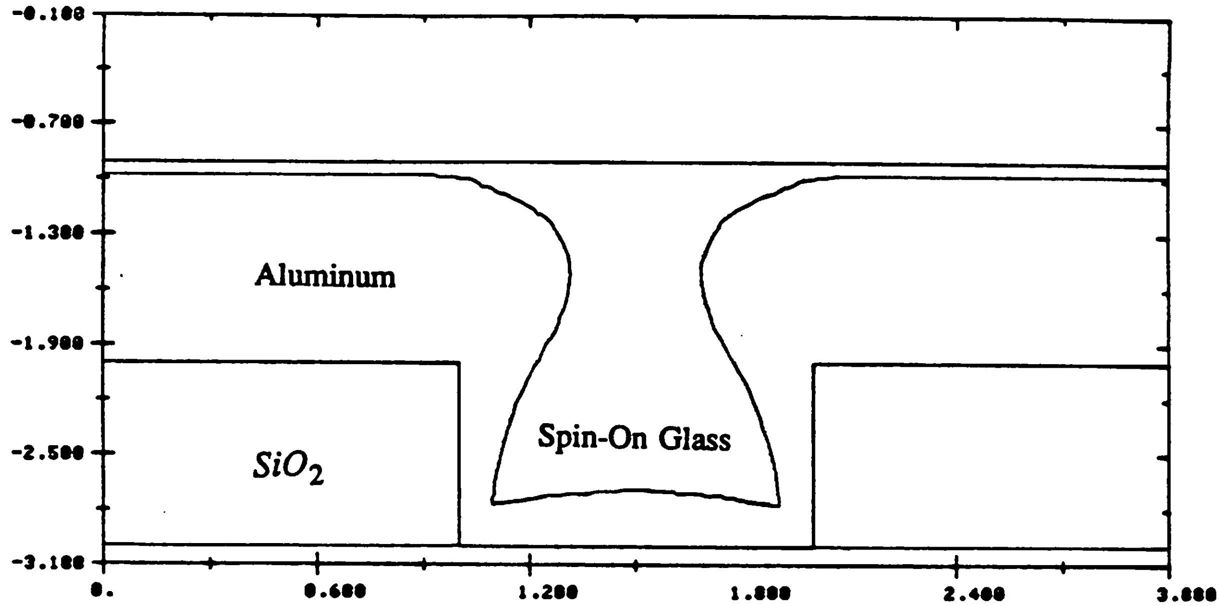


Figure 8: Etch of Top Spin-On Glass Layer

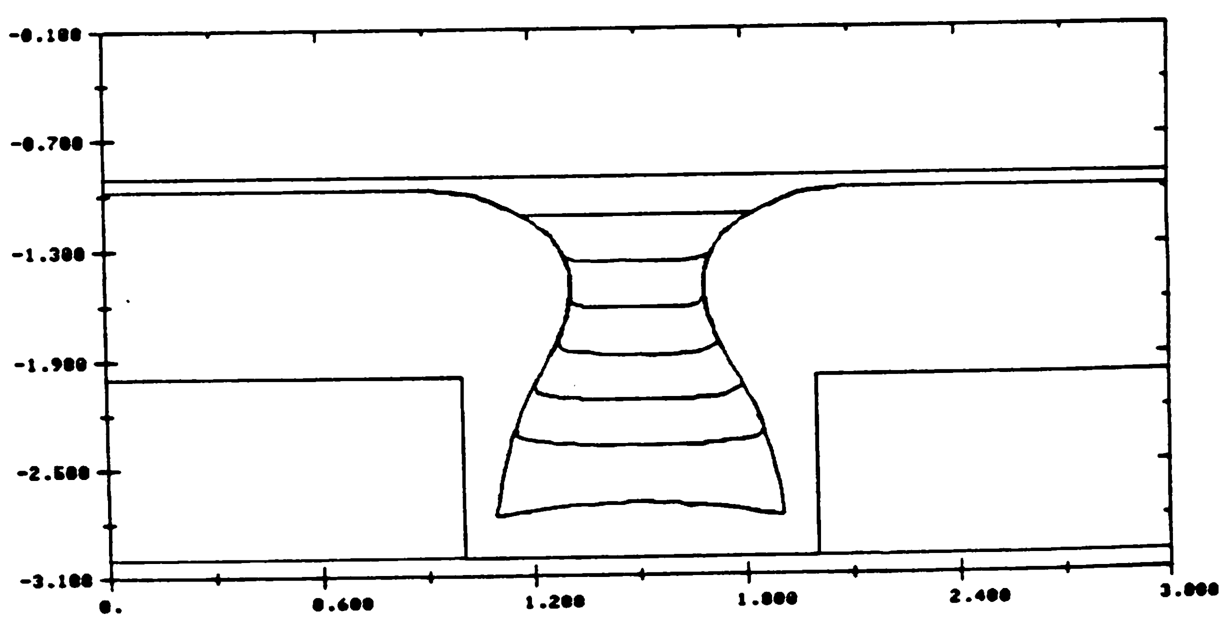
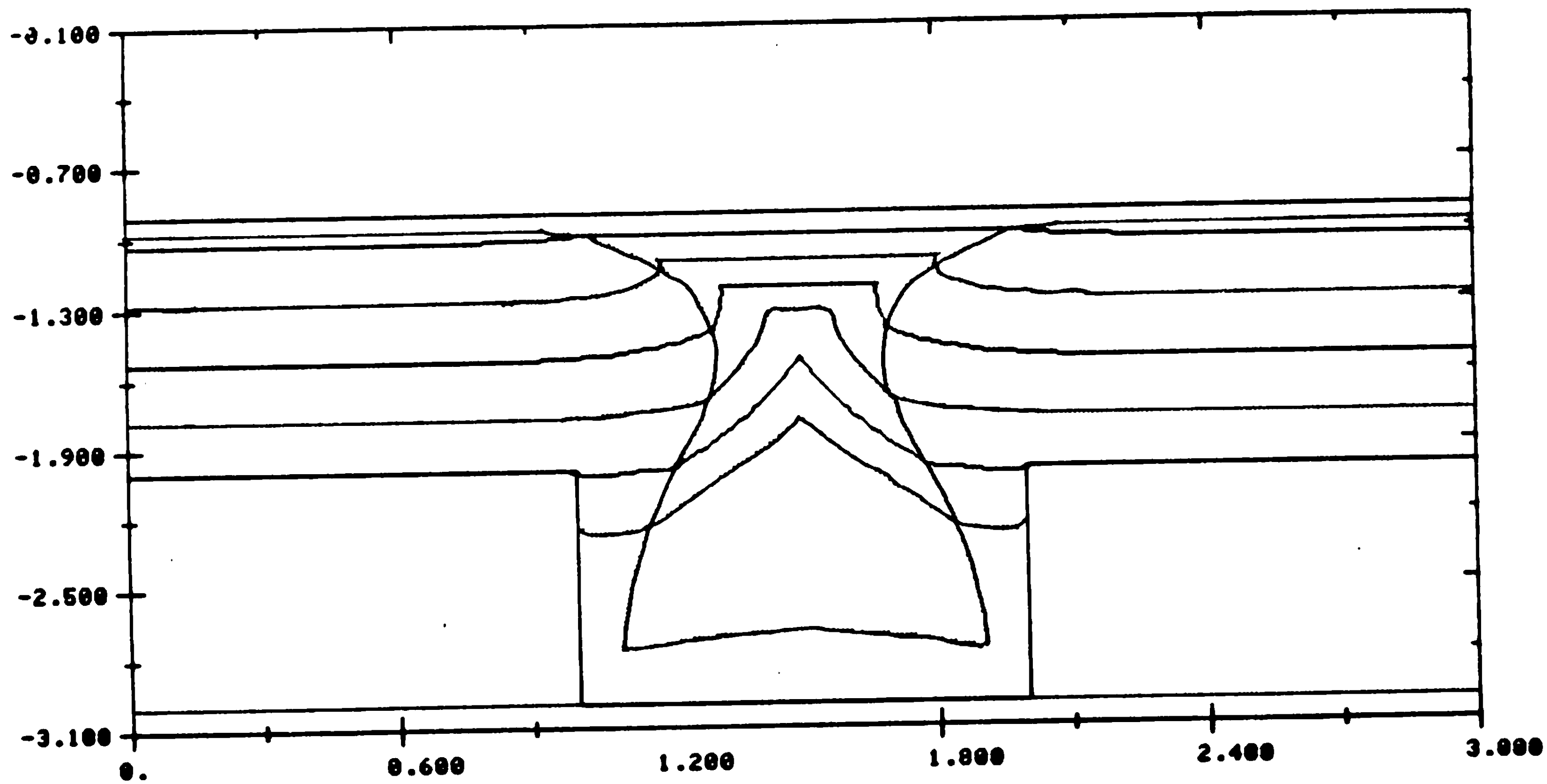


Figure 9: Simultaneous Etching of Spin-On Glass and Aluminum



Rates:

Spin–On Glass = .0015 $\frac{um}{sec}$

Aluminum = .0035 $\frac{um}{sec}$

Substrate = 0.0 $\frac{um}{sec}$

Figure 10: Oxide Spacer Process: Initial MOS Structure

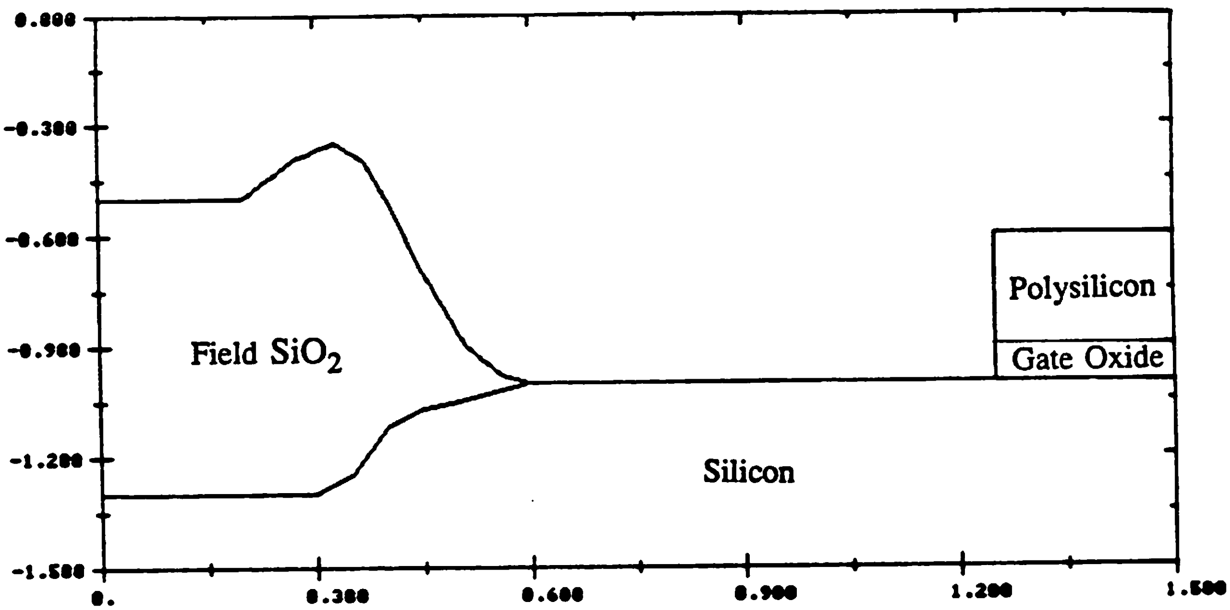


Figure 11: Spacer Process: Step #1 - Isotropic Deposition

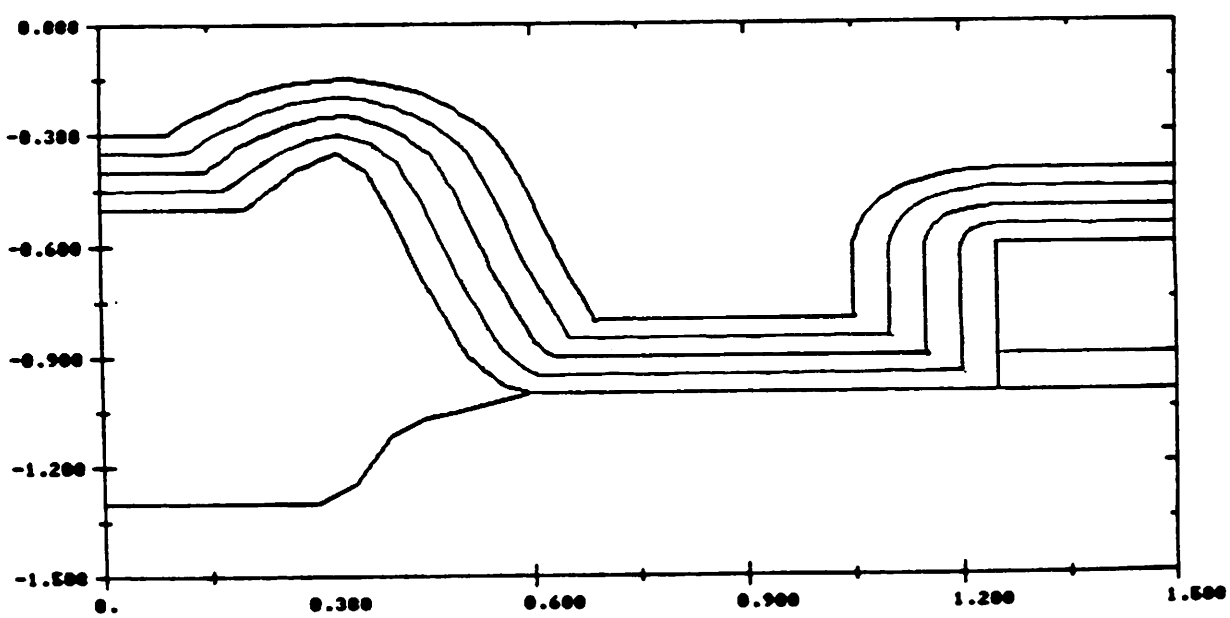


Figure 12: Spacer Process: Step #2 - Anisotropic Etch

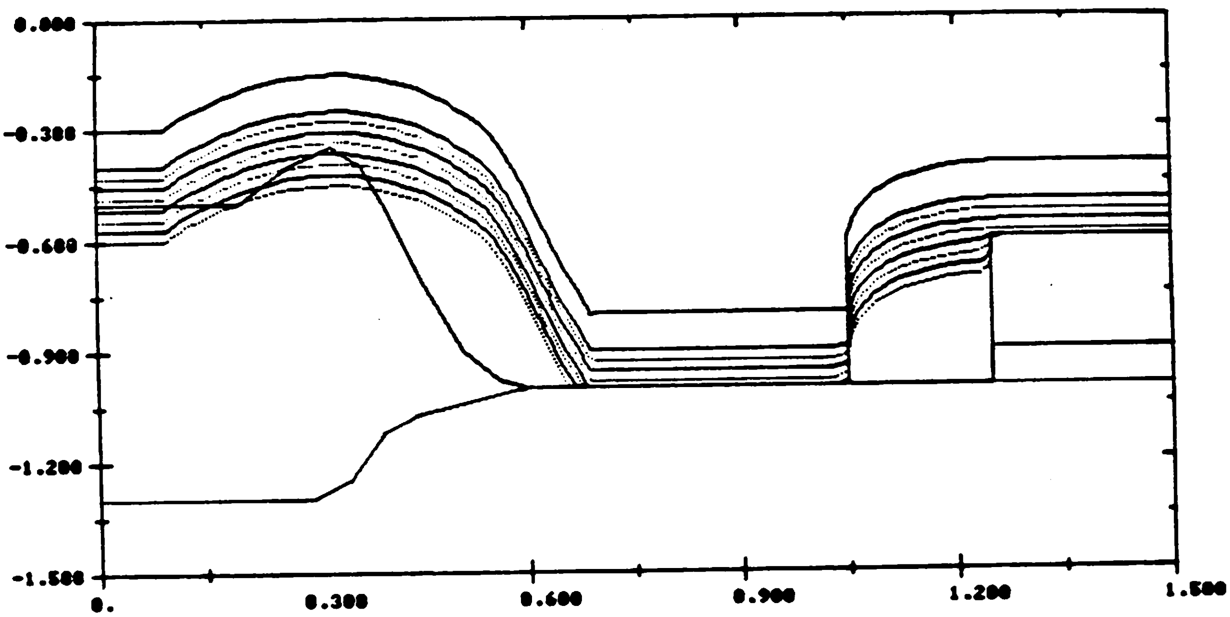


Figure 13: Spacer Process: Step #3 - Isotropic Etch

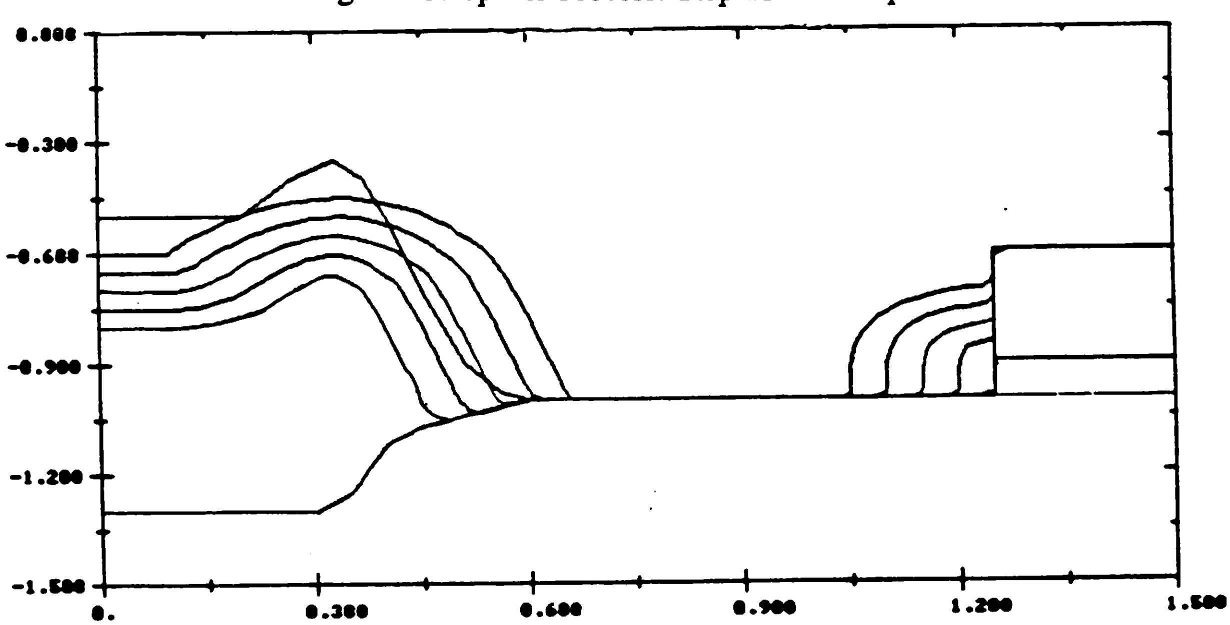


Figure 14: Initial Lift-Off Structure

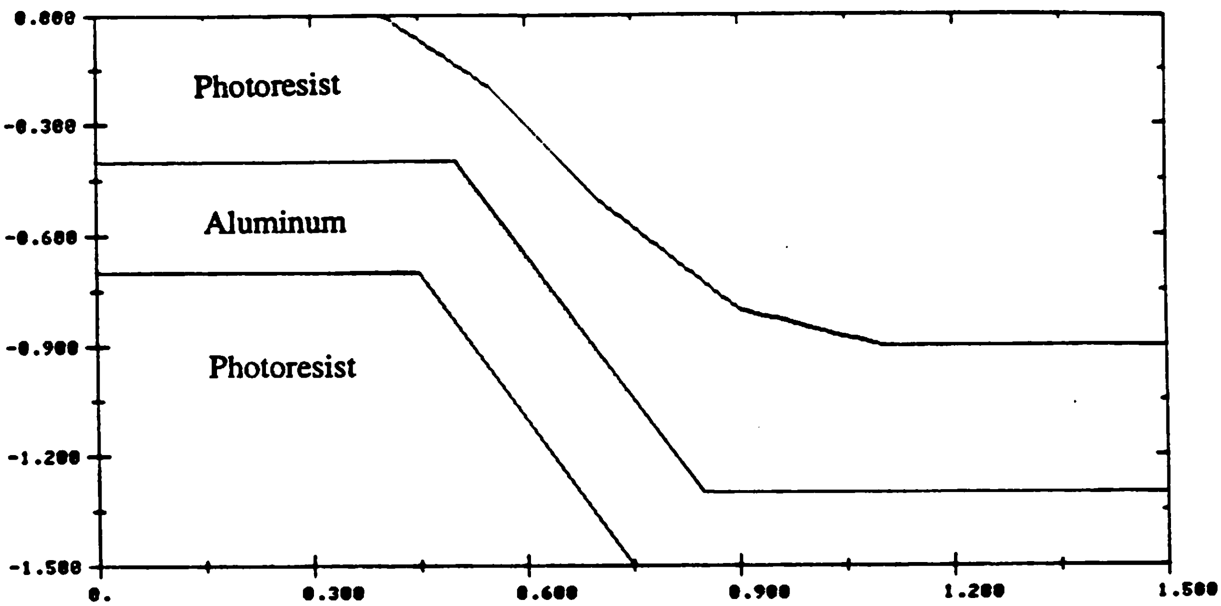


Figure 15: Etch of Top Photoresist Layer

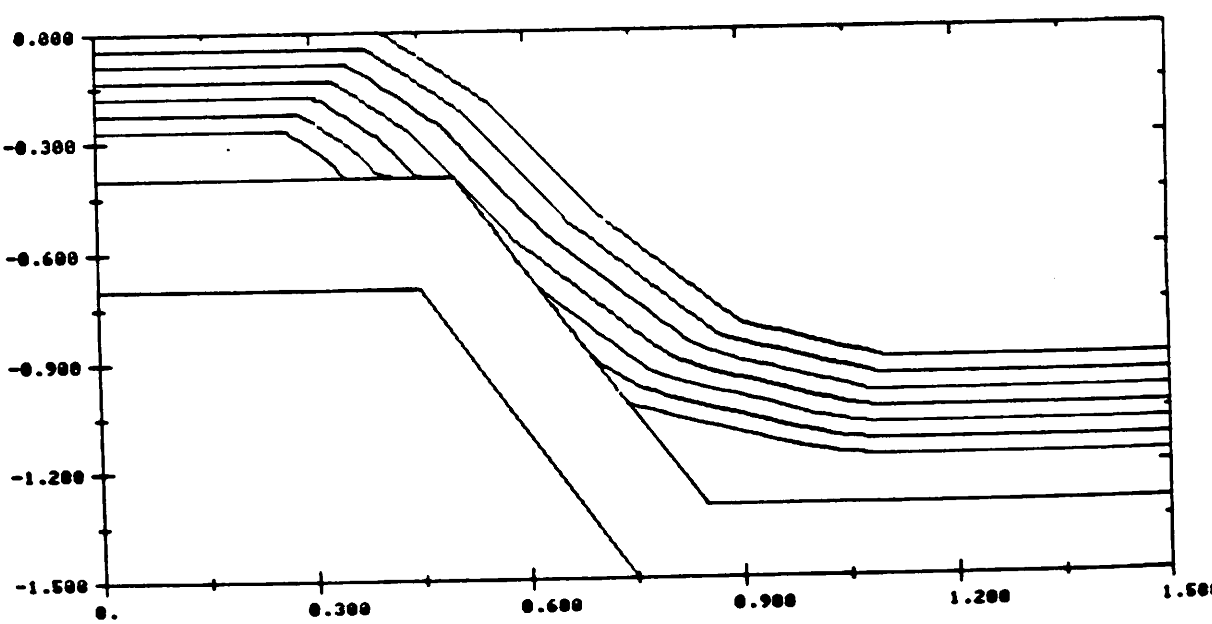


Figure 16: Etch of Aluminum Layer

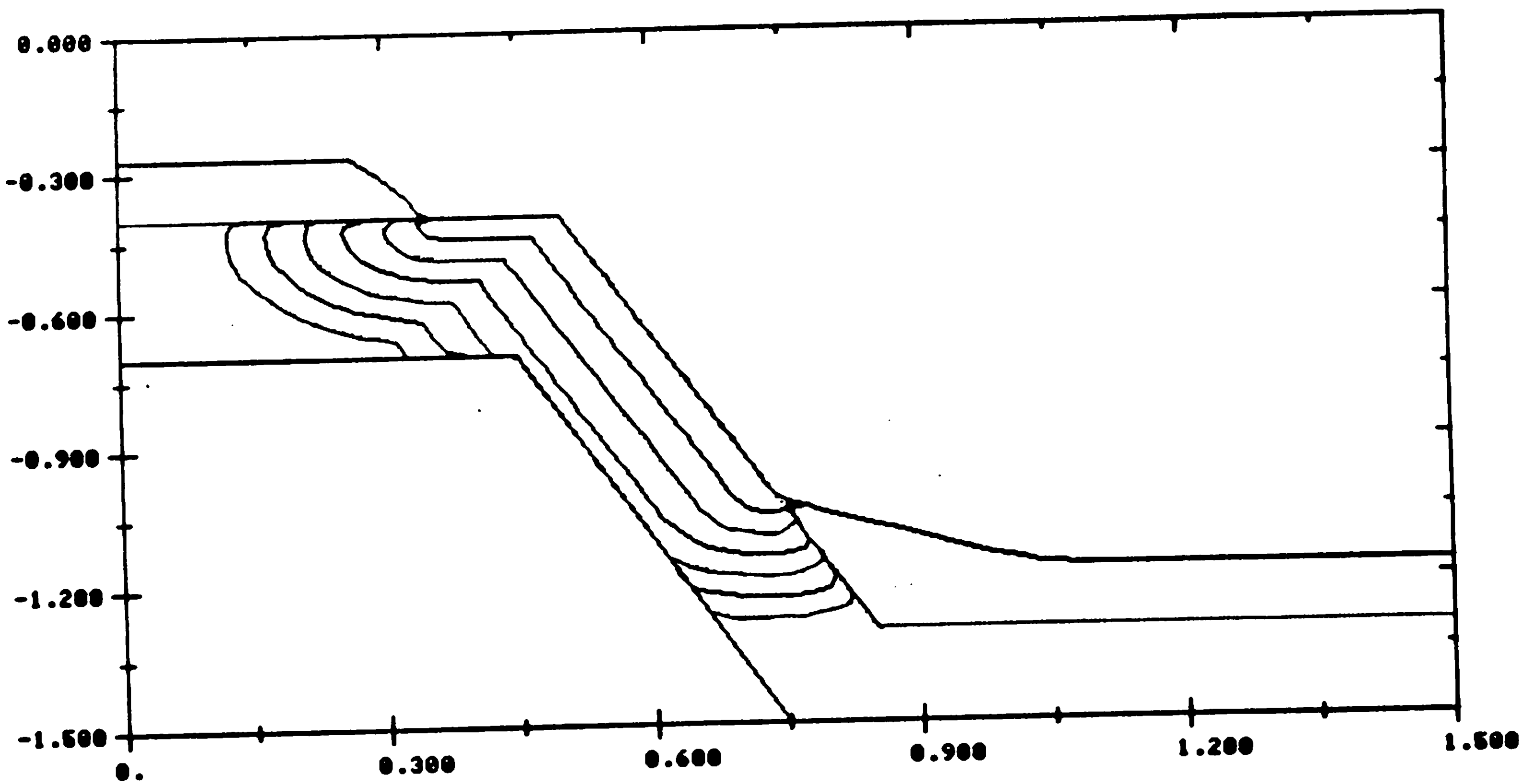


Figure 17: Initial Overhanging Lift-Off Structure

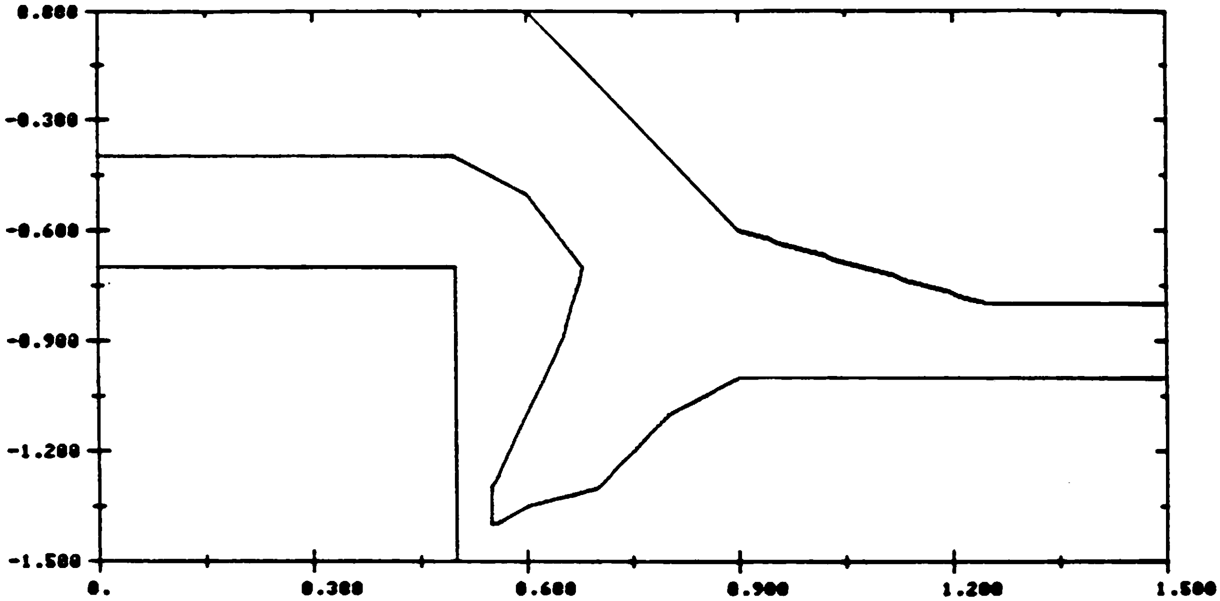


Figure 18: Etch of Top Photoresist Layer

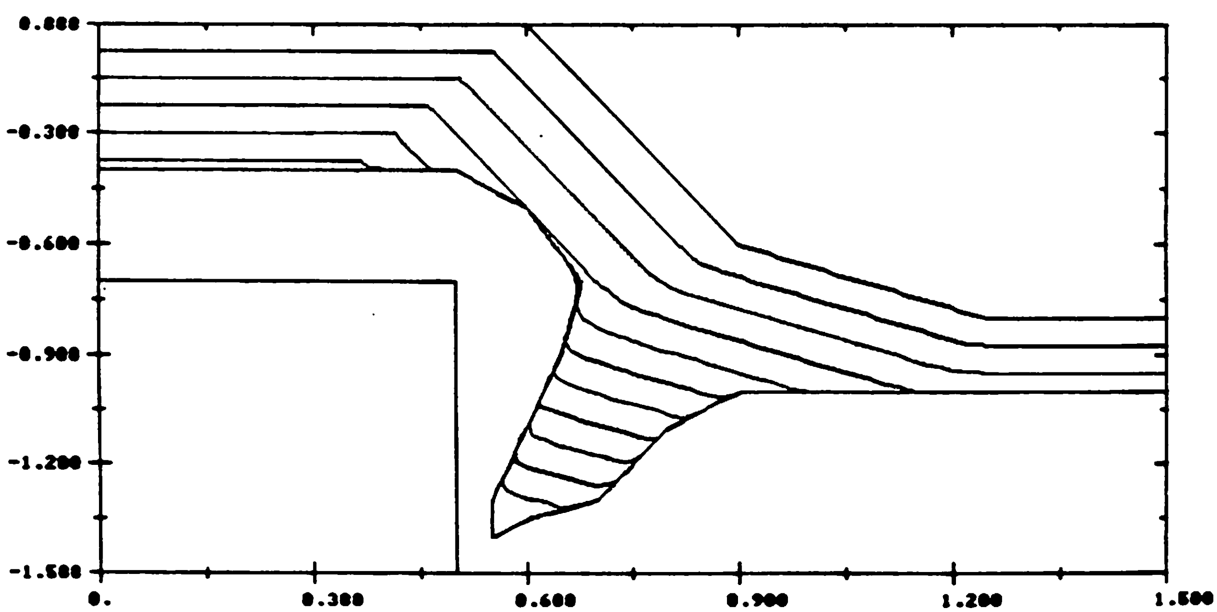
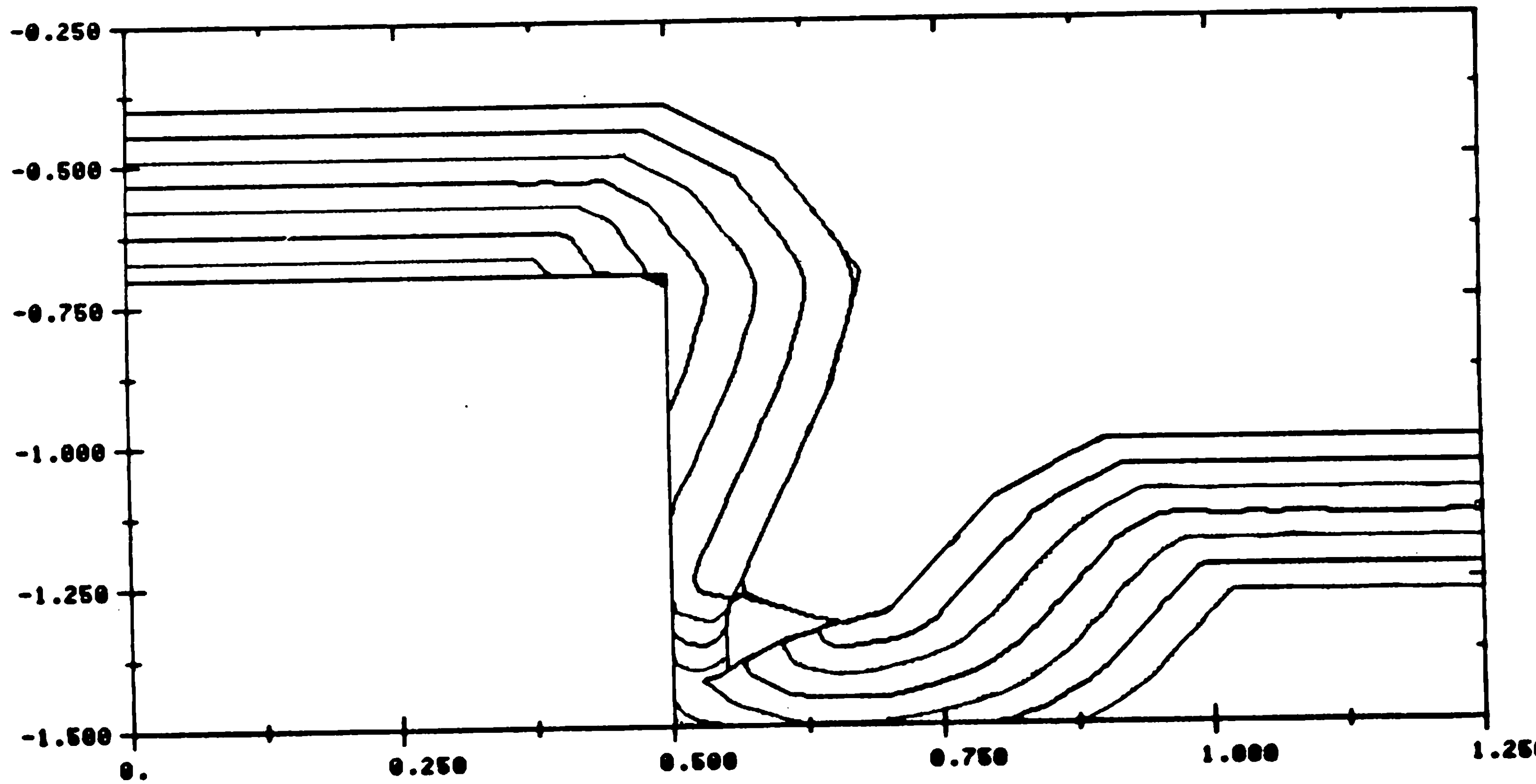


Figure 19: Etch of Aluminum Layer



Appendix

Input Files for Nonplanar Etching Examples

```
#-----------------------------------------------------------
# Non-Planar Etching example
# Example #1 - Spin-On and Etchback Planarization
#-----------------------------------------------------------
etchrates 1 0.0015 0.0015 0.0001 .0001 # Equal Matching of Rates
etchlayers -3 4 # Number of Layers = 4
#-----------------------------------------------------------
# Oxide Layer
#-----------------------------------------------------------
nonplanar 2 (0.0 .2) (.20 .2) (.25 .22) (.3 .3) (.35 .4) (.40 .6)
            (.85 .6) (.9 .4) (.95 .3) (1.0 .22) (1.05 .2) (1.25 .2)
#-----------------------------------------------------------
# Aluminum Layer
#-----------------------------------------------------------
nonplanar 1 (0.0 .7) (.30 .7) (.3 1.05) (.95 1.05) (.95 .7) (1.25 .7)
#-----------------------------------------------------------
# Substrate Layer
#-----------------------------------------------------------
nonplanar 0 (0.0 1.05) (1.25 1.05)
#-----------------------------------------------------------
# Photoresist Layer
#-----------------------------------------------------------
etchprof (0.0 0.0) (1.25 0.0)
etchaccur 8 1
etchwindow 1.25
etchtime 120 600 10
etchplot 1 0 0
etchrun
```

```
#--------------------------------------------------------
# Non-Planar Etching Example
# Example #2 - Oxide Spacer Formation Sequence
#--------------------------------------------------------
etchrates 2 -0.0005 -0.0005 -.0005 -.0005    # Isotropic Deposition
etchlayers -3 3
#--------------------------------------------------------
#  SiO2 Layer
#--------------------------------------------------------
nonplanar 1 (0.00 0.50) (0.20 0.50) (0.27 0.40) (0.33 0.35)
(0.37 0.40) (0.40 0.50) (0.45 0.70) (0.51 0.90)
(0.56 0.98) (0.60 1.00) (1.25 1.00) (1.25 0.90)
(1.50 0.90)
#--------------------------------------------------------
# Silicon Substrate
#--------------------------------------------------------
nonplanar 0 (0.00 1.30) (0.30 1.30) (0.35 1.25) (0.40 1.12)
(0.45 1.07) (0.50 1.05) (0.56 1.02) (0.60 1.00)
(1.50 1.00)
#--------------------------------------------------------
# Poly Layer
#--------------------------------------------------------
etchprof (0.00 0.50) (0.20 0.50) (0.27 0.40) (0.33 0.35)
(0.37 0.40) (0.40 0.50) (0.45 0.70) (0.51 0.90)
(0.56 0.98) (0.60 1.00) (1.25 1.00) (1.25 0.60)
(1.50 0.60)
etchaccur 12 1
etchwindow 1.5
etchtime 100 400 4
etchplot 1 0 0
etchrun
#--------------------------------------------------------
#  Anisotropic Etching
#  Note Number of Layers Automatically Increased by One
#--------------------------------------------------------
etchrates 10 (0.0 0.001667) (0.0 0.0) (0.0 0.00167) (0.0 0.0) (0.0 0.0)

etchwindow 1.5
etchtime 60 180 8
etchplot 1 0 0 1
etchrun
#--------------------------------------------------------
#  Isotropic Etching
#--------------------------------------------------------
etchrates 10 (.001667 0.0) (0.0 0.0) (0.00167 0.0) (0.0 0.0)
etchwindow 1.5
etchplot 1 0 0 1
etchtime 30 120 4
etchrun
```

```
*****************************************************
# Non-Planar Etching Example
# Example #3 - High Resolution Additive Lift-Off
#****************************************************
etchlayers -3 4              # Number of Layers = 4
#****************************************************
# Aluminum Layer
#****************************************************
nonplanar 2 (0.0 .4) (.5 .4) (.85 1.3) (1.25 1.3)
#****************************************************
# Second Photoresist
#****************************************************
nonplanar 1 (0.0 .7) (.45 .7) (.75 1.5) (1.25 1.5)
#****************************************************
# Substrate Layer
#****************************************************
nonplanar 0 (0.0 1.5) (1.25 1.5)
#****************************************************
# Top Photoresist Layer
#****************************************************
etchprof (0.0 0.0) (.40 0.0) (.55 .2) (.70 .5)
        (.9 .8) (1.1 .9) (1.25 .9)
etchaccur 8 1                  # Increase Accuracy
etchwindow 1.25                  # Window Size
#
#  Perform Etch of Top Photoresist Layer
#  Etch Top Only - Note: Rate of All Layers is Specified
#
etchrates 1 0.0015 0.000 0.000 .000
etchtime 30 180 6
etchplot 1 0 0
etchrun
#
#  Perform Etch of Aluminum Layer
#  Etch Second Only - Note: Rate of All Layers is Specified
#

etchtime 30 180 6
etchrates 1 0.000 0.0015 0.0000 .0000
etchplot 1 0 0 1
etchrun
```